# A new form for the third-order asymptotic aberration coefficients of electrostatic lenses; application to the two-tube electrostatic lens

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The third-order asymptotic aberration coefficients of round electrostatic lenses are reformulated in terms of the coordinates formed by the projections of the asymptotic incident and final rays onto the reference plane of the lens. In this formulation, all aberration coefficients are finite for all lenses, in contrast to the formulation in terms of coordinates projected onto the focal planes of the lenses, where all of the coefficients become infinite in the limit of very weak lenses and for certain strong lenses. Equations for the six third-order aberration coefficients are derived in the form of integrals involving derivatives of the axial potential no higher than the second. Using these equations and previously calculated potentials and first-order trajectories, we have computed the six aberration coefficients for the accelerating and decelerating two-tube electrostatic lens for voltage ratios from 1.1 to 10 000. The results are believed accurate to better than 0.2%.

#### INTRODUCTION

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In previous papers<sup>1,2</sup> we formulated the third-order asymptotic aberration coefficients<sup>3</sup> of round electrostatic lenses in terms of coordinates formed by the projections of the asymptotic incident and final rays onto the focal planes of the lens, derived integrals for the six third-order aberration coefficients, and presented results for the two-tube electrostatic lens for voltage ratios from 1.1 to 10 000. For the purpose of computer calculations of arbitrary systems of two-tube electrostatic lenses, these coefficients are unsuitable since they become infinite in the limit of very weak lenses and for certain strong lenses, causing difficulty in interpolating between the calculated coefficients. This be-

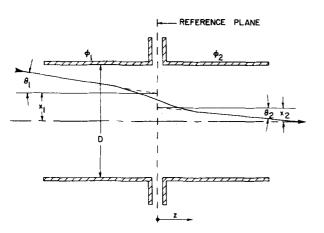


Fig. 1. Definition of the midplane coordinates of asymptotic rays. Note that  $\alpha_1 = \tan\theta_1$ ,  $\alpha_2 = \tan\theta_2$ , and that in the perpendicular plane we use  $y_1$ ,  $y_1$  and  $y_2$ ,  $y_2$ .

havior is a direct result of using ray coordinates projected onto the focal planes, since these coordinates also become infinite as the focal planes approach infinity. Hence a new formulation is desirable.

Such a new formulation of the aberration coefficients obviously requires that ray coordinates be used in planes near the lens. The most obvious and convenient choice is to use coordinates formed by the projections of the asymptotic incident and final rays onto the reference plane of the lens and for the two-tube lens, a plane midway between the two tubes of the lens. (Note that the reference plane could be at any convenient location. It is essential, however, that the first-order and third-order properties be expressed at the same plane.) This choice also allows us to make use of our formulation of the first-order properties of the electrostatic lens in terms of the same coordinates and of our calculations of these properties for the two-tube lens.<sup>4</sup>

In this paper we derive integrals for the new aberration coefficients and report results for the two-tube electrostatic lens at voltage ratios from 1.1 to 10 000.

### DEFINITION OF THE NEW ABERRATION COEFFICIENTS

The incident asymptotic ray is specified by its slopes  $\alpha_1$ ,  $\gamma_1$  and by its coordinates  $x_1$ ,  $y_1$  when projected onto the reference plane of the lens (the midplane for the two-tube lens, see Fig. 1). Similarly, the emerging asymptotic ray is specified by its slopes  $\alpha_2$ ,  $\gamma_2$  and by its coordinates  $x_2$ ,  $y_2$  when projected onto the reference plane of the lens. By asymptotic rays we mean rays outside of the effective

field of the lens; hence real objects must be outside of the lens field, otherwise, objects must be virtual. This is no real limitation since real objects cannot be placed in the field of an electrostatic lens without changing the properties of the lens.

Defining the dimensionless quantities  $X_1 = x_1/D$ ,  $Y_1 = y_1/D$ , and  $Z_1 = z_1/D$ , where D is the diameter of the lens, the coordinates are grouped as system invariants

$$r_1 = X_1^2 + Y_1^2 \qquad s_1 = \alpha_1^2 + \gamma_1^2 u_1 = X_1\alpha_1 + Y_1\gamma_1 \quad v_1 = X_1\gamma_1 - Y_1\alpha_1.$$
 (1)

The coefficient of  $v_1$  vanishes for electrostatic lenses.

Again following Hawkes<sup>5-7</sup> and our previous treatment<sup>1</sup> of aberration coefficients between the focal planes, the third-order properties are derived from a characteristic function  $V_F$  which is second order in  $r_1$ ,  $s_1$ ,  $u_1$ 

$$V_{F} = (r_{1} s_{1} u_{1}) \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ 0 & M_{22} & M_{23} \\ 0 & 0 & M_{33} \end{pmatrix} \begin{pmatrix} r_{1} \\ s_{1} \\ u_{1} \end{pmatrix}$$
(2)

We again deviate from Hawkes' formulation by defining  $V_F$  and the  $M_{ij}$  as dimensionless quantities. To derive the aberration equations, the following first-order trajectories G and H are required

$$G_1(Z) = 1$$
  $H_1(Z) = Z$   
 $G_1'(Z) = 0$   $H_1'(Z) = 1$ . (3)

The subscript 1 indicates projected values for the asymptotic incoming rays at the reference plane. Recalling<sup>4</sup> that the first-order properties of the lens in matrix form are given by

$$\binom{X_2}{\alpha_2} = \binom{a_{11}}{a_{21}} \frac{a_{12}}{a_{22}} \binom{X_1}{\alpha_1}, \tag{4}$$

where  $a_{11}a_{22}-a_{12}a_{21}=(\phi_1/\phi_2)^{\frac{1}{2}}$ , and  $\phi_1$ ,  $\phi_2$  are the asymptotic initial and final potentials of the lens, we find that the projected values for the asymptotic outgoing first-order rays are

$$G_2 = a_{11}$$
  $H_2 = a_{12}$   
 $G_2' = a_{21}$   $H_2' = a_{22}$ . (5)

The third-order (lateral) aberration equations are obtained from

$$\Delta X_{2} = H_{2} \frac{\partial V_{F}}{\partial X_{1}} - G_{2} \frac{\partial V_{F}}{\partial \alpha_{1}} - \frac{1}{2} H_{2} \alpha_{1} (\alpha_{1}^{2} + \gamma_{1}^{2}),$$

$$\Delta \alpha_{2} = H_{2} \frac{\partial V_{F}}{\partial X_{1}} - G_{2} \frac{\partial V_{F}}{\partial \alpha_{1}} - \frac{1}{2} H_{2} \alpha_{1} (\alpha_{1}^{2} + \gamma_{1}^{2}) + \frac{1}{2} \alpha_{2} (\alpha_{2}^{2} + \gamma_{2}^{2}),$$
(6)

where the quantities  $\alpha_2$ ,  $\gamma_2$  are first-order projected values, and equations for  $\Delta Y_2$ ,  $\Delta \gamma_2$  are obtained by replacing  $X_1$ ,  $\alpha_1$ ,  $\alpha_2$  with  $Y_1$ ,  $\gamma_1$ ,  $\gamma_2$ . Substituting the appropriate values of  $G_2$ ,  $G_2'$ ,  $H_2$ ,  $H_2'$  from Eqs. (5) and the first-order values

of  $X_2$ ,  $\alpha_2$  from Eq. (4), we find that to the third order

$$X_{2} = a_{11}X_{1} + a_{12}\alpha_{1} + a_{12}\frac{\partial V_{F}}{\partial X_{1}} - a_{11}\frac{\partial V_{F}}{\partial \alpha_{1}} - \frac{1}{2}a_{12}\alpha_{1}s_{1},$$

$$\alpha_{2} = a_{21}X_{1} + a_{22}\alpha_{1} + a_{22}\frac{\partial V_{F}}{\partial X_{1}} - a_{21}\frac{\partial V_{F}}{\partial \alpha_{1}} - \frac{1}{2}a_{22}\alpha_{1}s_{1}$$
(7)

 $+\frac{1}{2}(a_{21}X_1+a_{22}\alpha_1)(a_{21}^2r_1+2a_{21}a_{22}u_1+a_{22}^2s_1).$ 

From the definition of  $V_F$  we have

$$\frac{\partial V_F}{\partial X_1} = 4M_{11}X_1r_1 + 2M_{12}X_1s_1 + 2M_{13}X_1u_1 + M_{13}\alpha_1r_1 + M_{23}\alpha_1s_1 + 2M_{33}\alpha_1u_1,$$

$$+M_{23}\alpha_1s_1 + 2M_{33}\alpha_1u_1,$$

$$\frac{\partial V_F}{\partial \alpha_1} = M_{13}X_1r_1 + M_{23}X_1s_1 + 2M_{33}X_1u_1 + 2M_{12}\alpha_1r_1 + 4M_{22}\alpha_1s_1 + 2M_{22}\alpha_1u_1,$$
(8)

Equations (7) and (8) could now be combined to give  $X_2$ ,  $\alpha_2$  directly in terms of  $X_1$ ,  $\alpha_1$ ,  $r_1$ ,  $s_1$ ,  $u_1$  but calculations are simplified if Eqs. (7) and (8) are computed separately.

### **DERIVATION OF THE ABERRATION INTEGRALS**

Integrals for the quantities  $F_{ij}$  are obtained from the dimensionless characteristic function

$$V_F = \frac{1}{\phi_1^{\frac{1}{2}}} \int m^{(4)} dZ, \tag{9}$$

where  $m^{(4)}$  are the fourth-order terms in the expansion of

$$m = \phi^{\frac{1}{2}} (1 + X'^2 + Y'^2)^{\frac{1}{2}},$$
 (10)

and  $\phi(Z)$  is the axial potential distribution. Obtaining  $m^{(4)}$  from Grivet,<sup>8</sup> we have

$$V_{F} = \frac{1}{\phi_{1}^{\frac{1}{2}}} \int \phi^{\frac{1}{2}} \left\{ \frac{1}{128} \left[ \frac{\phi^{iv}}{\phi} - \left( \frac{\phi''}{\phi} \right)^{2} \right] (X^{2} + Y^{2})^{2} - \frac{1}{16} \frac{\phi''}{\phi} (X^{2} + Y^{2}) (\alpha^{2} + \gamma^{2}) - \frac{1}{8} (\alpha^{2} + \gamma^{2})^{2} \right\} dZ, \quad (11)$$

where  $\phi''$ ,  $\phi^{iv}$  are second and fourth derivatives of  $\phi$  with respect to Z. Note also that because we are calculating asymptotic properties at the reference plane, the integrals in Eqs. (9) and (11) are of the form

$$\int \equiv \int_0^{-\infty} + \int_{-\infty}^{\infty} + \int_{\infty}^{0} \tag{12}$$

where the first and last integral on the right involve only straightline asymptotic trajectories.

The integral in Eq. (11) must be evaluated for a general first-order trajectory, which may be expressed in terms of the trajectories G, H as follows

$$X = X_1G + \alpha_1H$$

$$Y = Y_1G + \gamma_1H$$

$$\alpha = X_1G' + \alpha_1H'$$

$$\gamma = Y_1G' + \gamma_1H'.$$
(13)

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Substituting Eqs. (13) into Eq. (11), we have

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$$V_{F} = \frac{1}{\phi_{1}^{1}} \int \phi^{\frac{1}{2}} \left\{ \frac{1}{128} \left[ \frac{\phi^{\text{iv}}}{\phi} - \left( \frac{\phi''}{\phi} \right)^{2} \right] (r_{1}G^{2} + 2u_{1}GH + s_{1}H^{2})^{2} \right.$$

$$\left. - \frac{1}{16} \frac{\phi''}{\phi} (r_{1}G^{2} + 2u_{1}GH + s_{1}H^{2}) (r_{1}G'^{2} + 2u_{1}G'H' + s_{1}H'^{2}) \right.$$

$$\left. - \frac{1}{8} (r_{1}G'^{2} + 2u_{1}G'H' + s_{1}H'^{2})^{2} \right\} dZ. \quad (14)$$

Before identifying the aberration coefficients the asymptotic contributions to  $V_F$  will be evaluated. Assume that the lens field is bounded by  $Z=L_1$  on the left and  $Z=L_2$  on the right. Then we can take

$$\int = \int_{0}^{L_{1}} + \int_{L_{2}}^{L_{2}} + \int_{L_{2}}^{0}.$$
 (15)

Note that the derivatives of  $\phi$  are zero in the first and last integral since the potential is constant outside of the lens field. Using Eqs. (5) and (3) to simplify the first and last integral, we obtain

$$V_{F} = \frac{1}{\phi_{1}^{\frac{1}{2}}} \int_{L_{1}}^{L_{2}} \phi^{\frac{1}{2}} \{ \} dZ - \frac{1}{8} L_{1} s_{1}^{2} + \frac{1}{8} L_{2} \left( \frac{\phi_{2}}{\phi_{1}} \right)^{\frac{1}{2}} \times (a_{21}^{2} r_{1} + 2a_{21} a_{22} u_{1} + a_{22}^{2} s_{1})^{2}.$$
 (16)

The term in braces is the same as in Eq. (14).

The aberration coefficients  $F_{ij}$  are now identified as appropriate terms of Eq. (16) by comparison with Eq. (2). They are identical in form with the equations we obtained previously for the asymptotic aberrations expressed between the focal planes [Eqs. (10) of Ref. 1] with the exception of the integrated terms, so we will not write them down here. Instead we will give equations for the aberration coefficients which have been transformed so that they contain no derivatives of the axial potential higher than the second order. The transformations are made exactly as in Ref. 1

$$\begin{split} M_{11} = & \frac{1}{\phi_1^{\frac{1}{2}}} \int_{L_1}^{L_2} \phi^{\frac{1}{2}} (KG^4 + LG^3G' + MG^2G'^2 + NG'^4) dZ \\ & + \frac{1}{8} \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} L_2 a_{21}^4, \\ M_{12} = & \frac{1}{\phi_1^{\frac{1}{2}}} \int_{L_1}^{L_2} \phi^{\frac{1}{2}} \left[ 2KG^2H^2 + L(G^2HH' + GG'H^2) \right. \\ & + M(4GG'HH' - G^2H'^2 - G'^2H^2) + 2NG'^2H'^2 \right] dZ \\ & + \frac{1}{4} \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} L_2 a_{21}^2 a_{22}^2, \\ M_{13} = & \frac{1}{\phi_1^{\frac{1}{2}}} \int_{L_1}^{L_2} \phi^{\frac{1}{2}} \left[ 4KG^3H + L(G^3H' + 3G^2G'H) \right. \\ & + 2M(G^2G'H' + GG'^2H) + 4NG'^3H \right] dZ \\ & + \frac{1}{2} \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} L_2 a_{21}^3 a_{22}, \end{split}$$

$$(17)$$

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$$M_{22} = \frac{1}{\phi_1^{\frac{1}{2}}} \int_{L_1}^{L_2} \phi^{\frac{1}{2}} (KH^4 + LH^3H' + MH^2H'^2 + NH'^4) dZ - \frac{1}{8}L_1 + \frac{1}{8} (\frac{\phi_2}{\phi_1})^{\frac{1}{2}} L_2 a_{22}^4,$$

$$\begin{split} M_{23} = & \frac{1}{\phi_1^{\frac{1}{2}}} \int_{L_1}^{L_2} \phi^{\frac{1}{2}} \Big[ 4KGH^3 + L(3GH^2H' + G'H^3) \\ & + 2M(GHH'^2 + G'H^2H') + 4NG'H'^3 \Big] dZ \\ & + \frac{1}{2} \Big( \frac{\phi_2}{\phi_1} \Big)^{\frac{1}{2}} L_2 a_{21} a_{22}^3, \end{split}$$

$$M_{33} = \frac{1}{\phi_1^{\frac{1}{3}}} \int_{L_1}^{L_2} \phi^{\frac{1}{3}} \left[ 4KG^2H^2 + 2L(G^2HH' + GG'H^2) + 2M(G^2H'^2 + G'^2H^2) + 4NG'^2H'^2 \right] dZ + \frac{1}{2} \left( \frac{\phi_2}{\phi_1} \right)^{\frac{1}{3}} L_2 a_{21}^2 a_{22}^2,$$

where

$$K = \frac{1}{512} \left( 3 \frac{\phi'' \phi'^2}{\phi^3} - 10 \frac{\phi''^2}{\phi^2} \right),$$

$$L = -\frac{3}{64} \frac{\phi'' \phi'}{\phi^2},$$

$$M = \frac{1}{32} \frac{\phi''}{\phi},$$

$$N = -\frac{1}{8}.$$
(18)

As in Ref. 2, there is a simple relationship, called Petzval's theorem, between  $M_{12}$  and  $M_{33}$ :

$$2M_{12} - M_{33} = -\frac{\phi_1^{\frac{1}{8}}}{8} \int_{L_1}^{L_2} \frac{\phi''}{\phi^{\frac{1}{8}}} dZ.$$
 (19)

## ABERRATION COEFFICIENTS FOR AN INVERTED LENS

Assuming now that we have carried out the calculation of the aberration coefficients  $M_{ij}$  for an accelerating lens, we would like to obtain the aberration coefficients of the inverted (decelerating) lens without the necessity of reevaluating the integrals of Eqs. (17). In the case of asymptotic aberration coefficients between the focal planes, there is a very simple relationship between the coefficients of an accelerating lens and those of the corresponding decelerating lens, and vice versa. In the present formulation, the relationship is more complicated.

To derive the relationships between the aberration coefficients of a given lens and those of the inverted lens, we start with Eqs. (17) rewritten for the inverted lens. For example, the first aberration coefficient of the inverted lens is given by

$$M_{11}^{i} = \frac{1}{\phi_{2}^{i}} \int_{-L_{2}}^{-L_{1}} \phi^{*\frac{1}{2}} (K^{*}\tilde{G}^{4} + L^{*}\tilde{G}^{3}\tilde{G}' + M^{*}\tilde{G}^{2}\tilde{G}'^{2} + N^{*}\tilde{G}'^{4}) dZ^{*} - \frac{1}{8} (\frac{\phi_{1}}{\phi_{1}})^{\frac{1}{2}} L_{1}b_{21}^{4}, \quad (20)$$

where  $Z^* = -Z$ ,  $\phi^*$ ,  $K^*$ ,  $L^*$ ,  $M^*$ ,  $N^*$  are for the inverted lens,  $b_{21}$  is a matrix element of the inverted lens, and  $\tilde{G}$ ,

 $\tilde{G}', \tilde{H}, \tilde{H}'$  are trajectories defined as

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$$\tilde{G}_1(Z^*) = 1$$
  $\tilde{H}_1(Z^*) = Z$   $\tilde{G}_1'(Z^*) = 0$   $\tilde{H}_1'(Z^*) = 1$ , (21)

where the subscript 1 again indicates projected values for the incoming rays of the inverted lens at the reference plane. Equation (20) is now transformed to be a function of Z,

$$M_{11}^{i} = \frac{1}{\phi_{2}^{\frac{3}{2}}} \int_{L_{1}}^{L_{2}} \phi^{\frac{1}{2}} (K\bar{G}^{4} - L\bar{G}^{3}\bar{G}' + M\bar{G}^{2}\bar{G}'^{2} + N\bar{G}'^{4}) dZ - \frac{1}{8} (\frac{\phi_{1}}{\phi_{2}})^{\frac{1}{2}} L_{1}b_{21}^{4}. \quad (22)$$

Finally, we make the substitutions

$$\tilde{G} = \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} (a_{22}G - a_{21}H),$$

$$\tilde{H} = \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} (a_{12}G - a_{11}H),$$

$$b_{21} = \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} a_{21},$$
(23)

expand the integrand, and collect terms to identify contributions from the integrals of Eq. (17). [Actually this process was performed on the simpler integrals analogous to Eqs. (10) of Ref. 2.] After much tedious but elementary algebra, we arrive at

$$\begin{split} M_{11}^{\mathrm{i}} = & \left(\frac{\phi_2}{\phi_1}\right)^{\frac{3}{2}} \left[a_{22}^{4} M_{11} - a_{21} a_{22}^{3} M_{13} + a_{21}^{2} a_{22}^{2} (M_{12} + M_{33}) \right. \\ & - a_{21}^{3} a_{22} M_{23} + a_{21}^{4} M_{22}\right], \\ M_{12}^{\mathrm{i}} = & \left(\frac{\phi_2}{\phi_1}\right)^{\frac{3}{2}} \left[2a_{12}^{2} a_{22}^{2} M_{11} - a_{12} a_{22} (a_{11} a_{22} + a_{12} a_{21}) M_{13} \right. \\ & + (a_{11}^{2} a_{22}^{2} + a_{12}^{2} a_{21}^{2}) M_{12} + 2a_{11} a_{12} a_{21} a_{22} M_{33} \\ & - a_{11} a_{21} (a_{11} a_{22} + a_{12} a_{21}) M_{23} + 2a_{11}^{2} a_{21}^{2} M_{22}\right], \\ M_{13}^{\mathrm{i}} = & \left(\frac{\phi_2}{\phi_1}\right)^{\frac{3}{2}} \left[4a_{12} a_{22}^{3} M_{11} - a_{22}^{2} (a_{11} a_{22} + 3a_{12} a_{21}) M_{13} \right. \\ & + 2a_{21} a_{22} (a_{11} a_{22} + a_{12} a_{21}) (M_{12} + M_{33}) - a_{21}^{2} (3a_{11} a_{22} + a_{12} a_{21}) M_{23} + 4a_{11} a_{21}^{3} M_{22}\right], \\ M_{22}^{\mathrm{i}} = & \left(\frac{\phi_2}{\phi_1}\right)^{\frac{3}{2}} \left[a_{12}^{4} M_{11} - a_{11} a_{12}^{3} M_{13} + a_{11}^{2} a_{12}^{2} (M_{12} + M_{33}) \right. \\ & - a_{11}^{3} a_{12} M_{23} + a_{11}^{4} M_{22}\right], \\ M_{23}^{\mathrm{i}} = & \left(\frac{\phi_2}{\phi_1}\right)^{\frac{3}{2}} \left[4a_{12}^{3} a_{22} M_{11} - a_{12}^{2} (3a_{11} a_{22} + a_{12} a_{21}) M_{13} \right. \\ \end{split}$$

$$\begin{split} +2a_{11}a_{12}(a_{11}a_{22}+a_{12}a_{21})(M_{12}+M_{33})-a_{11}^2(a_{11}a_{22}\\ +3a_{12}a_{21})M_{23}+4a_{11}^3a_{21}M_{22}],\\ M_{33}^i =& \left(\frac{\phi_2}{\phi_1}\right)^{\frac{1}{2}} \left[4a_{12}^2a_{22}^2M_{11}-2a_{12}a_{22}(a_{11}a_{22}+a_{12}a_{21})M_{13}\\ +4a_{11}a_{12}a_{21}a_{22}M_{12}+(a_{11}a_{22}+a_{12}a_{21})^2M_{33}-2a_{11}a_{21}\\ \times (a_{11}a_{22}+a_{12}a_{21})M_{23}+4a_{11}^2a_{21}^2M_{22}\right]. \end{split}$$

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### TRANSFORMATIONS BETWEEN MIDPLANE AND FOCAL-PLANE ABERRATION COEFFICIENTS

Finally, we wish to derive the transformations between the midplane and focal-plane aberration coefficients. We begin with Eqs. (7) and (8). Denoting by  $\xi$  and  $\eta$  the position coordinates in the initial focal plane, and by  $R_1$ ,  $S_1$ ,  $U_1$  the corresponding system invariants, we make the substitutions

$$X_{1} = -\frac{1}{a_{21}}(\xi_{1} + a_{22}\alpha_{1}),$$

$$Y_{1} = -\frac{1}{a_{21}}(\eta_{1} + a_{12}\alpha_{2}),$$

$$r_{1} = \frac{1}{a_{21}^{2}}(R_{1} + 2a_{22}U_{1} + a_{22}^{2}S_{1}),$$

$$s_{1} = S_{1},$$

$$u_{1} = -\frac{1}{a_{21}}(U_{1} + a_{22}S_{1}),$$

$$X_{2} = -\frac{a_{11}a_{22} - a_{12}a_{21}}{a_{21}}\xi_{2} + \frac{a_{11}}{a_{21}}\alpha_{2}.$$
(25)

After considerable algebraic manipulation, we can identify the focal plane aberration coefficients,  $F_{ij}$ , which have the following form<sup>2</sup>:

$$-\xi_{2} = \alpha_{2} + 4F_{11}\xi_{1}R_{1} + 2F_{12}\xi_{1}S_{1} + 2F_{13}\xi_{1}U_{1} + F_{13}\alpha_{1}R_{1} + (F_{23} - \frac{1}{2})\alpha_{1}S_{1} + 2F_{33}\alpha_{1}U_{1},$$

$$\alpha_{2} = -\xi_{1} + (F_{13} - \frac{1}{2})\xi_{1}R_{1} + F_{23}\xi_{1}S_{1} + 2F_{33}\xi_{1}U_{1} + 2F_{12}\alpha_{1}R_{1} + 4F_{22}\alpha_{1}S_{1} + 2F_{23}\alpha_{1}U_{1}.$$

$$(26)$$

We find that

We find that
$$F_{11} = -\frac{1}{a_{21}^{3}} M_{11} - \frac{1}{8} \frac{a_{11}}{a_{11}a_{22} - a_{12}a_{21}},$$

$$F_{12} = -\frac{2a_{22}^{2}}{a_{21}^{3}} M_{11} - \frac{1}{a_{21}} M_{12} + \frac{a_{22}}{a_{21}^{2}} M_{13},$$

$$F_{13} = -\frac{4a_{22}}{a_{21}^{3}} M_{11} + \frac{1}{a_{21}^{2}} M_{13},$$

$$F_{22} = -\frac{a_{22}^{4}}{a_{21}^{3}} M_{11} - \frac{a_{22}^{2}}{a_{21}} M_{12} + \frac{a_{22}^{3}}{a_{21}^{2}} M_{13} - a_{21} M_{22} + a_{22} M_{23} \qquad (27)$$

$$-\frac{a_{22}^{2}}{a_{21}} M_{33} - \frac{1}{8} a_{22},$$

$$F_{23} = -\frac{4a_{22}^{3}}{a_{21}^{3}} M_{11} - \frac{2a_{22}}{a_{21}} M_{12} + \frac{3a_{22}^{2}}{a_{21}^{2}} M_{13} + M_{23} - \frac{2a_{22}}{a_{21}} M_{33},$$

$$F_{33} = -\frac{4a_{22}^{2}}{a_{23}^{3}} M_{11} + \frac{2a_{22}}{a_{21}^{2}} M_{13} - \frac{1}{a_{21}^{2}} M_{33}.$$

The Eqs. (27) can easily be solved to give the M's in terms

TABLE I. Accelerating midplane aberration coefficients.

$\phi_2/\phi_1$	$M_{11}$	$M_{12}$	$M_{13}$	$M_{22}$	$M_{23}$	$M_{33}$
1.1	-8.3949 - 4	-4.3653 - 4	1.9770 - 5	-2.3146 -5	5.8111 -3	5.6689 -4
1.3	-6.0764 -3	-3.2258 -3	3.8731 - 4	-1.6499 - 4	1.5435 2	4.0090 - 3
1.5	-1.3908 -2	-7.5334 - 3	1.3521 - 3	-3.8579 - 4	2.3248 - 2	9.0072 - 3
2	-3.6938 - 2	-2.1020 -2	6.0610 - 3	-1.1237 -3	3.8312 - 2	2.3146 - 2
5	-1.3304 - 1	-9.8097 - 2	5.5014 - 2	-7.4219 -3	9.1413 - 2	7.5737 - 2
10	-1.8410 -1	-1.8343 -1	1.3179 - 1	-1.9427 -2	1.5373 - 1	8.6976 - 2
20	-2.0751 - 1	-2.9037 - 1	2.5079 - 1	-4.2714 - 2	2.5588 - 1	4.2970 - 2
40	-2.2180 - 1	-4.1847 - 1	4.1727 - 1	-8.3468 -2	4.1531 - 1	-6.9239 - 2
100	-2.4427 - 1	-6.1032 - 1	6.7909 - 1	-1.7781 - 1	7.3195 - 1	-3.0717 - 1
250	-2.6101 - 1	-8.1421 - 1	9.2306 - 1	-3.4617 - 1	1.1988	-6.1388 - 1
500	-2.6581 - 1	-9.8383 - 1	1.0883	-5.5409 - 1	1.7028	-8.9974 - 1
1000	-2.6829 - 1	-1.1814	1.2577	-8.6263 - 1	2.3904	-1.2567
2000	-2.7335 - 1	-1.4169	1.4490	-1.2977	3.2967	-1.6995
5000	-2.8140 - 1	-1.7703	1.7139	2.0968	4.8177	-2.3812
6600	-2.8353 - 1	-1.8841	1.7928	-2.3961	5.3501	-2.6033
9000	-2.8555 - 1	-2.0146	1.8791	-2.7668	5.9868	-2.8589
0 000	-2.8616 - 1	-2.0599	1.9081	-2.9021	6.2137	-2.9478

of the F's. We find

$$M_{11} = -a_{21}{}^{3}F_{11}^{*},$$

$$M_{12} = -2a_{21}a_{22}{}^{2}F_{11}^{*} - a_{21}F_{12} + a_{21}a_{22}F_{13}$$

$$M_{13} = -4a_{21}^2a_{22}F_{11}^* + a_{21}^2F_{13}$$

$$M_{22} = \frac{1}{a_{21}} (-a_{22} {}^{4}F_{11} {}^{*} - a_{22} {}^{2}F_{12} - a_{22} {}^{3}F_{13} - F_{22} + a_{22}F_{23}$$
(28)

$$M_{23} = -4a_{22}{}^{3}F_{11}^{*} - 2a_{22}F_{12} + 3a_{22}{}^{2}F_{13} + F_{23} - 2a_{22}F_{33}$$

$$M_{33} = -4a_{21}a_{22}{}^{2}F_{11}^{*} + 2a_{21}a_{22}F_{13} - a_{21}F_{33}$$

where

$$F_{11}^* = F_{11} + \frac{1}{8} \frac{a_{11}}{a_{11}a_{22} - a_{12}a_{21}}$$

### **EVALUATION OF THE ABERRATION INTEGRALS**

The aberration integrals of Eqs. (17) were evaluated for the two-tube electrostatic lens for voltage ratios (accelerating) from 1.1 to 10 000. Potentials were calculated with a precision of 1 in 10<sup>5</sup> using overrelaxation on a 593×81 network covering the entire lens. Trajectories were calculated using the predictor-corrector method. Details of these methods have already been given<sup>9</sup> together with applica-

tions to first-order focal properties<sup>10-12</sup> and matrix elements<sup>18</sup> of the two-tube electrostatic lens.

Paraxial trajectories G were already available from the previous calculations,  $^{10-12}$  needing only to be suitably scaled to satisfy Eqs. (3). New paraxial trajectories H were calculated for use in the aberration integrals. Axial potentials were calculated using five-point Lagrange interpolation between the five closest mesh points. Derivatives of the axial potential were obtained from the interpolating polynomial.

The integrals giving the six aberration coefficients were calculated using the Romberg iterative method.<sup>13</sup> This method uses "cautious extrapolation" from results on two or more intervals and gives error estimates. In our calculations the integrals were required to converge to a precision of better than 0.1% which necessitated division of each mesh interval into 16 points ( $\Delta z = D/1080$ , where D is the diameter of the lens.)

#### **RESULTS AND DISCUSSION**

Results for the six aberration coefficients for accelerating lenses with voltage ratios from 1.1 to 10 000 are given in Table I. Coefficients for decelerating lenses were calculated from Eqs. (24) using matrix elements from Ref. 4, and are given in Table II. The behavior of the aberration coeffi-

TABLE II. Decelerating midplane aberration coefficients.

$\phi_1/\phi_2$	M <sub>11</sub> i	$M_{12}^{i}$	$M_{13}{}^{\mathrm{i}}$	M 22 <sup>i</sup>	$M_{23}$ i	M 83i
1.1	-8.8043 - 4	-4.4885 - 4	-2.1425 - 5	-2.4703 - 5	-6.0943 -3	6.1250 -
1.3	-6.9291 -3	-3.4824 -3	-4.8291 -4	-1.9726 -4	-1.7581 - 2	4.9622 -
1.5	-1.7050 -2	-8.4757 -3	-1.9026 -3	-5.0736 -4	-2.8360 - 2	1.2533 —
2	-5.2522 -2	-2.5661 - 2	-1.0904 - 2	-1.7722 -3	-5.3074 $-2$	4.0863 —
5	-3.0814 - 1	-1.5556 -1	-2.1707 - 1	-1.8009 - 2	-1.5398 - 1	2.9694 —
10	-5.5709 - 1	-3.8149 - 1	-8.5577 - 1	-5.3304 - 2	-2.0507 - 1	6.7221 —
20	-4.6223 - 1	-8.9167 - 1	-2.1548	-1.1104 - 1	-1.7451 -1	1.0060
40	6.9898 —1	-1.9426	-3.3604	-1.8734 - 1	-1.7552 -1	9.7016 —
100	4.4055	-3.9785	-5.0463	-3.7221 -1	-6.5072 -1	1.1780
250	7.1213	-4.8642	1.0740	-6.9603 -1	-2.6028 -1	6.3130
500	4.3664	-4.3811	1.8189 +1	-5.6415 -1	3.8092	1.5118 +
1000	-2.9666	-6.1749	1.5126 +1	9.2702 —1	1.1801 +1	2.2638 +
2000	-1.1251 +1	-0.1749 -1.4773 +1	3.1883	4.4656		
5000	-2.2134 + 1	-3.3588 + 1	-3.3695		1.6984 +1	2.1184 +
6600	-2.6876 +1	-3.7786 + 1		9.9183	-1.0928 -1	1.4794 +
9000	-2.0670 + 1 -3.3131 + 1	-3.7780 + 1 -4.0159 + 1	-3.4122 7.5060	1.0637 + 1	-1.1658 + 1	1.9056 +
0 000			-7.5868 1.0067 1.1	1.0452 + 1	-2.6162 +1	3.0692 +
10 000	-3.5285 + 1	-4.0422 +1	-1.0967 + 1	1.0067 + 1	-3.0902 +1	3.6334

cients as a function of the voltage ratio is shown in Fig. 2. For accelerating lenses the coefficients vary more smoothly than for decelerating lenses, although  $M_{11}$  and  $M_{13}$  show some structure. Because of the strong cancellations which occur in the calculation of  $M_{13}$  at a voltage ratio of 6600, the pronounced structure in this region may not be real.

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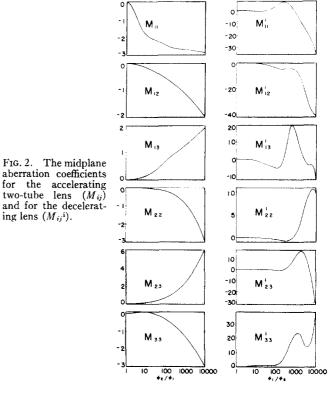
There is no definitive way to estimate the accuracy of the aberration coefficients and no previous data for direct comparison. The axial potentials, first-order trajectories and matrix elements are believed to be accurate to better than 0.1%,4.11 and as discussed above, the integrals were evaluated to a precision of better than 0.1%. The precision of the calculations can be demonstrated by testing our values against Petzval's theorem, Eq. (19). For all lenses, both accelerating and decelerating, this relation is satisfied to an accuracy of better than about 0.04%. We believe that the numerical calculation of derivatives of the axial potential introduces errors less than 0.1%, because our previous calculation<sup>14</sup> of focal-plane aberration coefficients using two forms of the aberration integrals gave agreement to better than 0.1%. We believe that a conservative estimate of the accuracy of the midplane aberration coefficients is 0.2%, and that they are sufficiently accurate for any practical calculations.

A further test of precision has been made by using Eqs. (27) to calculate the focal-plane aberration coefficients from the midplane aberration coefficients. The agreement is typically much better than 0.01% except for isolated values at voltage ratios of 100 and 250 where it is better than 0.3%, and is obtained using both the accelerating and decelerating coefficients. It is interesting to note that converting focal-plane aberration coefficients to midplane aberration coefficients with Eqs. (28) generally gives less accuracy, particularly in the weak and very strong lenses, because of strong cancellations which occur. Thus the midplane aberration coefficients have the additional advantage of being more suitable for calculating other aberration coefficients.

From the complete set of third-order aberration coefficients which we have presented here for the two-tube electrostatic lens, it is possible to calculate the position and slope to third-order of the exit trajectory which corresponds to any incident ray. Since skew trajectories are included, it would be possible to calculate spot diagrams in analogy with similar calculations in light optics. 15 Furthermore, the coefficients are in a form which is ideal for the calculation of aberrations of lens systems, and are sufficiently wellbehaved for convenient numerical representation for computer calculations.

The derivation of equations to calculate the more usual coefficients of spherical aberration, coma, astigmatism, curvature of field, and distortion from the midplane aberration coefficients will be the subject of a future paper. Similar equations for the focal-plane aberration coefficients have been given by Verster<sup>16</sup> and Hawkes.<sup>6</sup>

Finally, we have presented a new set of aberration integrals with which it is possible to calculate all of the aberra-



tions of an electrostatic lens, given only the axial potential and two first-order trajectories. Since the new aberration coefficients have been shown to be preferable to any previous coefficients, it is hoped that the availability of these integrals will encourage similar calculations for other electrostatic lenses.

#### **ACKNOWLEDGMENT**

We thank Annija Galejs for carrying out many of the numerical tests of the aberration coefficients.

\*Work supported by Consiglio Nazionale delle Ricerche under Italy-USA cooperative program.

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